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Hot electron transmission in metals using epitaxial $NiSi_2$/n-Si(111) interfaces

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We have investigated hot electron transmission across epitaxial metal-disilicide/n-Si(111) interfaces using ballistic electron emission microscopy (BEEM). Different crystal orientations of epitaxial $NiSi_2$ were grown on a Si(111) substrate using molecular beam epitaxy. The presence of different interfaces of $NiSi_2$ on Si(111) were confirmed by high resolution transmission electron microscopy. Electrical transport measurements reveal a clear rectifying Schottky interface with a barrier height of 0.69 eV. However, using BEEM, three different regions with different transmissions and Schottky barrier heights of 0.65 eV, 0.78 eV, and 0.71 eV are found. The addition of a thin Ni film on the $NiSi_2$ layer strongly reduces the transmission in all the three regions and interestingly, almost equalizes the transmission across them. © *2011 American Institute of Physics*. [doi:10.1063/1.3610458]

Spin injection and detection of electrons in semiconductor spintronic devices has been recently demonstrated,[1,2] based on the hot electron transport scheme. It was shown that the efficiency of electron spin transport in bulk silicon (Si), in such devices, is reduced by the presence of undesirable and uncontrollable silicides at the ferromagnet (FM)/Si interface.[2] On the other hand, properly tuned epitaxial silicides can be grown on Si substrates with enhanced thermal stability and such interfaces can be used as building blocks of semiconductor spintronic devices. Such epitaxial interfaces, which can be tuned to grow atomically abrupt on Si, are also an ideal model system to study spin transport in general.

To study electron transport across a buried metal/semiconductor (M/S) interface with nanometer scale resolution, relevant for designing nanoscale spintronic devices, and to investigate lateral non-uniformities in transmission, ballistic electron emission microscopy (BEEM) (Ref. 3) is a very suitable technique. Based on hot electrons, BEEM is a non-destructive technique that can be used to probe local Schottky barrier height (SBH) inhomogeneities with high spatial resolution,[4] to study spin-dependent transport in metal and organic spin valves across polycrystalline M/S interface, in determining the attenuation lengths in several material systems, in magnetic imaging etc.[5–9]

In BEEM, hot electrons are injected from the tip of a scanning tunneling microscope (STM) into a thin metallic film grown on a semiconducting substrate. Depending on the scattering in the metal layer, a fraction of the hot electrons propagate to the M/S interface, where they can be collected as BEEM current, I_B, provided they satisfy the necessary energy and momentum criteria to overcome the SBH at that interface. From I_B, measured at different local regions, SBH can be determined on the local (nanometer) scale using Bell-Kaiser (BK) model.[3]

In order to use such epitaxial interfaces for studying spin-dependent transmission in spin-valve structures, it is first necessary to investigate hot electron transmission across the M/S interface. In this work, hot electron transmission on carefully grown epitaxial interfaces of $NiSi_2$/n-Si(111) has been studied. By tuning the initial Ni thickness and the annealing temperature, three distinctly different interfaces of $NiSi_2$ on n-Si(111) are observed in BEEM studies with varying BEEM transmission. This result closely matches with theoretical calculations done for ballistic transport in such systems,[10] for which no experimental evidence existed thus far. Adding a thin capping layer of Au does not reduce I_B significantly, however, the insertion of a thin Ni layer between Au and $NiSi_2$ does. It strongly reduces the BEEM transmission at all interfaces and interestingly, makes the transmission almost equal for all. We analyze our results by considering the differences in transmission probabilities at the different epitaxial M/S interfaces and the influence of inelastic and elastic scattering of hot electrons in polycrystalline metallic layers as Au and Ni on such epitaxial interfaces.

For this study, epitaxial $NiSi_2$ films were grown on Si(111) substrates in an ultra high vacuum molecular beam epitaxy (UHV MBE) system following the well established method of Tung *et al.*[11] Substrates consist of buffered hydrofluoric acid (HF)-etched n-Si(111) with a lithographically defined area of 150 μm diameter, surrounded by thick SiO_2 insulator.[9] The Si surface was H-terminated using 1% HF and immediately loaded into MBE system, at a base pressure of 10^{-10} mbar. A pre-annealing step at 550 °C for 5 min was done before depositing Ni of thickness ~1.5 nm at room temperature (RT). The temperature of the substrate was thereafter raised to 500 °C for 5 min to form $NiSi_2$. The thickness of the $NiSi_2$ layer is 2–3.5 times the deposited Ni layer thickness. Further deposition of the top Ni layer (3 nm) on $NiSi_2$/Si(111) and the Au cap layer (4 nm) were done at RT. The devices were then transferred into an UHV STM system and BEEM measurements were performed at RT. A large area ohmic back contact to n-Si(111) is used to collect the transmitted hot electrons, I_B, while the top metal overlayer is grounded [see inset of Fig. 2(a)].

The growth of $NiSi_2$ layer on Si(111) is studied using cross-sectional high resolution transmission electron

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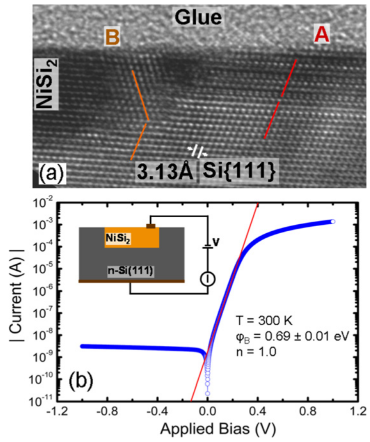

FIG. 1. (Color online) (a) High-resolution TEM images of thin $NiSi_2$ film on Si(111) substrate viewed along $\langle 1\bar{1}0 \rangle$ direction. The $NiSi_2$ film is formed on Si(111) surface as described in the text. Type A and Type B regions are clearly visible. (b) Electrical (I-V) characterization of $NiSi_2$/n-Si(111) Schottky interface of the above structure at RT. The straight line is a fit using the thermionic emission theory as described in the text.

microscopy (HRTEM) and shown in Fig. 1(a). Two different crystal orientations of $NiSi_2$ on Si(111) are possible by tuning the deposited Ni thickness and the annealing temperature.[11] When the lattice of $NiSi_2$ is aligned along the direction of the underlying Si(111) lattice, the interface is called Type-A; when they are 180° rotated about the Si surface normal, the interface is called Type-B.[11] The lattice mismatch is about 0.46%.[11] The details of the growth and formation of the different interfaces is explained elsewhere.[11] Figure 1(a) shows the co-existence of both Type A and Type B interface with an intermediate region. Differences in local thickness of the initial Ni layer and their growth kinetics can lead to the coexistence of such different interfaces.

The $NiSi_2$/n-Si(111) interface is first characterized using standard current-voltage (I-V) measurements. Figure 1(b) shows a typical I-V characteristic. At RT, clear rectifying behavior, with low reverse leakage current is observed with the forward bias current increasing rapidly with increasing bias. The barrier height was obtained from the I-V plot by fitting the forward bias characteristics using the thermionic emission theory

$$I = A^{**}.A.T^2.exp\left(-\frac{q\phi_B}{k_B T}\right)\left[exp\left(-\frac{qV}{nk_B T}\right) - 1\right] \quad (1)$$

The symbols have their usual meanings.[12] The extracted SBH of the $NiSi_2$/n-Si(111)interface is 0.69 ± 0.01 eV with an ideality factor 1.

Hot electron transmission in epitaxial $NiSi_2$/n-Si(111) interface is studied using BEEM. Representative BEEM spectra, shown in Fig. 2(a), are obtained by sweeping the tip bias while recording I_B at constant tunnel current injection. Each spectrum is an average of more than 100 individual spectra taken at several different locations of the device. With increasing tip bias, a rather sharp onset of I_B is observed which corresponds to the local Schottky barrier height at the M/S interface. Three distinct regions corresponding to three M/S interfaces are found with different BEEM transmission. The local Schottky barrier heights are

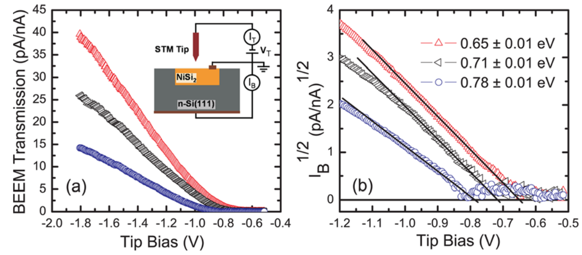

FIG. 2. (Color online) (a) BEEM transmission per nA of injected tunnel current in $NiSi_2$/Si(111) layer, at RT, of the same device as in Fig. 1(b). Three different regions with different values of transmitted current are measured. Inset shows the schematic of the BEEM technique. The STM tip locally injects electrons into the sample by tunneling at bias voltage V_T between tip and $NiSi_2$ layer. The current I_B transmitted perpendicularly through the layer is collected in n-Si with a third electrical contact at the rear. (b) Square root of the BEEM transmission with applied bias in V_T. The intercepts of the solid lines with the voltage axis give the local Schottky barrier heights for the three interfaces according to BK model.

extracted, using BK model,[3] by plotting the square root of I_B with tip bias V [see Fig. 2(b)]:

$$\frac{I_B}{I_T} \propto (V_T - \phi_B)^2. \quad (2)$$

Near threshold, the intercepts of the solid lines with the voltage axis yields SBHs of 0.65 ± 0.01 eV, 0.71 ± 0.01 eV, and 0.78 ± 0.01 eV corresponding to Type A, intermediate and Type B interfaces,[11] respectively. Unlike the macroscopic I-V characteristic [Fig. 1(b)] yielding a single SBH, BEEM measurements on the same sample reveals three different SBHs. This establishes the sensitivity of the BEEM to probe local inhomogeneities in electron transport on the nanoscale. From the BEEM spectra, it is seen that I_B for Type A interface is ~3 times larger than for Type B whereas the transmission for the intermediate phase lies in between. The hot electron transmission and collection at the M/S interface is sensitive to the inelastic and elastic scattering in the $NiSi_2$ layer as well as to the details of the electronic structure and bonding of Ni and Si at the interface. The 3 times larger transmission at Type A interface than at Type B, which has not been earlier observed, matches well with a theoretical work by Stiles and Hamann[10] They find that a factor of 3 difference in transmission is not due to the difference in the Schottky barrier heights at the different interfaces but due to a difference in the transmission probabilities across them. The Type A lattice, which is in perfect registry with the underlying Si lattice reflects >50% of the incident electrons whereas the Type B interface, which is rotated 180° with Si(111) lattice, reflects the incident electrons even more strongly (>80%).[10] Assuming the inelastic scattering in the $NiSi_2$ layer to be the same for all the crystal orientations, this difference in transmission probability causes the reduction in I_B that we observe between Type A and Type B interface. This reduction is quite surprising, given the fact that the structure of the two interfaces differ only in the position of the third and highest nearest neighbors. Whether such differences in transmission probabilities arises due to an incompletely bonded Ni (Type B) or a fully bonded Si (Type A),[10] or due to the absence of matching states at either side of the interface, or due to strain is difficult to conjecture at this point.

Further, we have also studied BEEM transmission across these three interfaces by adding a thin polycrystalline Au layer (4 nm) on $NiSi_2$ [Fig. 3(a)]. The BEEM transmission is reduced at Type A interface from 39 pA to 30 pA (at −1.8 eV), from 26 pA to 20 pA at the intermediate interface and from 14 pA to 8 pA at Type B interface. I_B can be described as[13]

$$I_B \propto T_{Au} T_{NiSi_2} \propto \alpha . \left[exp\left(-\frac{d_{Au}}{\lambda_{Au}}\right) exp\left(-\frac{d_{NiSi_2}}{\lambda_{NiSi_2}}\right)\right], \qquad (3)$$

where the transmission $T_{Au,NiSi_2}$ depends exponentially on the hot electron attenuation length (λ) in the films of thicknesses (d) and on the transmission across the interfaces (α). The attenuation length of hot electrons in Au, at −1.8 eV, is quite large (~12 nm);[14] thus, a thin Au film does not attenuate I_B significantly, as is also observed [Fig. 3(a)]. The nominal reduction in I_B at all the three interfaces is due to the interfacial attenuation at polycrystalline Au and epitaxial $NiSi_2$ interface. The interfacial attenuation is a combination of the mismatch of the electronic states at both sides of the interface and elastic scattering due to interface disorder, defects, etc.[7,13]

However, the insertion of a thin polycrystalline Ni layer (3 nm) between Au and $NiSi_2$ layer strongly reduces the transmission at all the interfaces [Fig. 3(b)]. The reduction in I_B is strongest at Type A and intermediate interface (~4–5 times) but less at Type B interface (~2.5 times). No noticeable changes to the Schottky barrier heights are observed at all the three interfaces as compared to Fig. 2(a). I_B can now be written as

$$I_B \propto T_{Au} T_{Ni} T_{NiSi_2} \propto \beta . \left[exp\left(-\frac{d_{Au}}{\lambda_{Au}}\right) exp\left(-\frac{d_{Ni}}{\lambda_{Ni}}\right) exp\left(-\frac{d_{NiSi_2}}{\lambda_{NiSi_2}}\right)\right]. \qquad (4)$$

Thus, I_B now depends also on the hot electron attenuation (both elastic and inelastic) in Ni in addition to that in Au and attenuation at their corresponding interfaces (β). Attenuation at the Au/Ni interface is expected to be minimal (good match of the electronic band structure),[15] but strong inelastic and elastic scattering in bulk Ni and elastic scattering at the non-epitaxial Ni/$NiSi_2$ interface increases the fraction of the incident electrons that do not have the necessary energy and momentum required to reach the underlying Si(111), thus decreasing the overall transmission. In a recent study,[16] we have found the hot electron attenuation length in Ni to be ~3 nm. Thus, the introduction of a 3 nm Ni layer should reduce

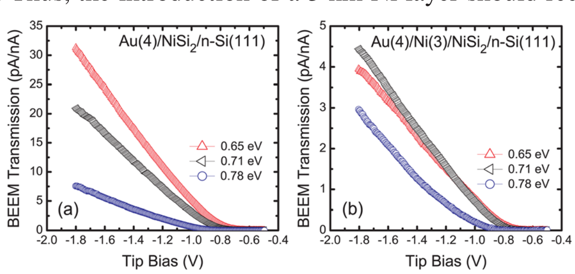

FIG. 3. (Color online) (a) BEEM transmission per nA of injected tunnel current in Au (4nm)/$NiSi_2$/Si(111)layer stack. The transmission is different at all the interfaces and only nominally decreased as compared to Fig. 2(a). Data is taken at RT. (b) BEEM transmission per nA of injected tunnel current in Au (4nm)/Ni (3 nm)/$NiSi_2$/Si(111) layer stack. The transmission decreases significantly due to inelastic scattering in the Ni layer and at the two interfaces.

I_B at all the interfaces, at least, by a factor of *e*. This is the case at Type B interface. However, the reduction in I_B at Type A and intermediate interface is much stronger. Interestingly, the transmission at all the three interfaces is now almost equal. This is most likely due to a reduced transmission probability at Type A interface as compared to Type B. Further experiments with different combinations of polycrystalline layers/epitaxial interfaces are needed to obtain further insights into this.

The epitaxial $NiSi_2$/Si(111) interface is a unique model system to investigate the role of inelastic and elastic scattering to electron transport. Epitaxial interfaces of $NiSi_2$ with different crystal orientations on Si(111) were prepared and confirmed by HRTEM studies. Although standard I-V characteristic yields a single SBH for this structure, local BEEM studies show the presence of three clear regions. Local transport measurements using BEEM reveal a larger transmission at the Type A interface than at the Type B interface. This observation closely matches with a theoretical calculation done for such interfaces. Addition of a thin Ni layer capped with Au is found to decrease the transmission at all the interfaces, primarily due to the increased inelastic scattering in the Ni layer. Electronic band structure calculation of $NiSi_2$ along with a quantification of the inelastic scattering length in differently oriented $NiSi_2$ will be useful to design spin valve devices with such interfaces.

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